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NEWS
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         MAR 31
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                  applications updated
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         MAR 31
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         JUN 13
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                 CA/CAplus enhanced with printed Chemical Abstracts
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                 CAOLD to be discontinued on December 31, 2008
NEWS 29
         AUG 15
                 CAplus currency for Korean patents enhanced
NEWS 30
         AUG 25
                 CA/CAplus, CASREACT, and IFI and USPAT databases
                  enhanced for more flexible patent number searching
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FULL ESTIMATED COST

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chain nodes:
9 10
ring nodes:
1 2 3 4 5 6 7 8
chain bonds:
1-9 9-10
ring bonds:
1-2 1-7 2-3 3-4 4-5 4-8 5-6 6-7 7-8
exact/norm bonds:
1-2 1-7 1-9 2-3 3-4 4-5 4-8 7-8 9-10
exact bonds:
5-6 6-7
isolated ring systems:
containing 1:

G1:0,S,N

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sss full FULL SEARCH INITIATED 16:38:13 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 73 TO ITERATE

100.0% PROCESSED 73 ITERATIONS 47 ANSWERS SEARCH TIME: 00.00.15

L2 47 SEA SSS FUL L1

=> fil cap COST IN U.S. DOLLARS SINCE FILE TOTAL FULL ESTIMATED COST ENTRY SESSION 178.36 178.57

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FILE COVERS 1907 - 26 Aug 2008 VOL 149 ISS 9 FILE LAST UPDATED: 25 Aug 2008 (20080825/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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L3 10 L2

=> d 1-10 abs ibib hitstr

L3 ANSWER 1 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

AB Although it is accepted that trifluoroacetic acid (TFA) can cause suppression of an analyte during LC/MS anal., this paper presents a relatively sensitive gradient method that uses a TFA mobile phase for the improved quantification of small, polar drug-like compds. The described method was developed in a discovery drug metabolism and pharmacokinetics (DMPK) laboratory for the screening measurement of compound concns. to calculate PK

parameters and CNS exposure of compds. from a chemical series that had poor chromatog. under generic methods using formic acid mobile phase. The samples were collected by a Culex automated sampling unit, and the plasma proteins were precipitated by a Tecan robot in 96-well plates. After centrifugation, the supernatant was removed, dried down using a SPE-Dry unit, and the samples were reconstituted in aqueous buffer on the robot. The samples were analyzed on an Agilent LC/MSD using a 5-min gradient on a 5 cm Ph column. No addnl. steps, such as the "TFA-fix", were necessary. Although sample batches were analyzed over 6 h, no drift or degradation of signal was observed. The improved chromatog. resulted in a method that was selective, rugged, and had a dynamic range from 5 to 20,000 nM, which was sufficient to quantitate low volume, serial plasma samples collected out to 8 h postdose.

ACCESSION NUMBER: 2007:996358 CAPLUS

DOCUMENT NUMBER: 147:461507

TITLE: Use of trifluoroacetic acid to quantify small, polar

compounds in rat plasma during discovery-phase

pharmacokinetic evaluation

AUTHOR(S): Bock, M. J.; Neilson, K. L.; Dudley, A.

CORPORATE SOURCE: Discovery DMPK, AstraZeneca, Wilmington, DE, 19803,

USA

SOURCE: Journal of Chromatography, B: Analytical Technologies

in the Biomedical and Life Sciences (2007), 856(1-2),

165-170

CODEN: JCBAAI; ISSN: 1570-0232

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal LANGUAGE: English

IT 857521-69-8

RL: ANT (Analyte); PKT (Pharmacokinetics); ANST (Analytical study); BIOL (Biological study)

(use of trifluoroacetic acid to quantify small, polar compds. in rat plasma during discovery-phase pharmacokinetic evaluation)

RN 857521-69-8 CAPLUS

CN Methanone, (1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-yl[5-(3-pyridinyl)-2-oxazolyl]- (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN GI

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ N & & & \\ N & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ &$$

AB Title compds. I [wherein X = N, CR2, P = CR3, Q = CR4; R = CR5; W = CR6, or one of P, Q, R, W = N; R1, R2 = independently <math>H, alkyl; R3, R4, R5, R6

= independently H, halo, alkyl, alkoxy, NO2, NH2 and derivs., CF3, CN, NHCO2H and derivs., OH and derivs., SH and derivs., CO2H and derivs., CONH2 and derivs., etc.; R3CCR4, R4CCR5, R5CCR6 = (un)substituted hetero/aromatic 6-membered; their free bases and salts of addition with acids] were prepared as CNS agents, and specifically as ligands of nicotinic receptor. The compds. were tested against nicotinic receptors with the $\alpha 4\beta 2$ subunit or with the $\alpha 7$ subunit. Thus, reacting 3-iodo-6-chloro-1H-indazole with 1,4-diazabicyclo[3.2.1]octane and CO in the presence of TEA/DMF at 70° for 8 h gave II \bullet HCl (m.p. = 285-286°). In tests for specific binding to isolated rat cerebral nicotinic receptors having either $\alpha 4\beta 2$ or $\alpha 7$ subunits, compds. I displayed IC50 values in the ranges of 1-10 μ M and 0.01-0.1

2005:637812 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 143:133407

TITLE: Preparation of 1,4-diazabicyclo[3.2.1]octanecarboxamid

 μM , resp. I showed selectivity for the $\alpha7$ receptor subtype.

es as ligands for nicotinic receptors, especially

 $\alpha 4\beta 2$ and $\alpha 7$ subunits, for treating central nervous system diseases

Galli, Frederic; Leclerc, Odile; Lochead, Alistoir W. INVENTOR(S):

PATENT ASSIGNEE(S): Sanofi-Synthelabo S.A., Fr.

SOURCE: Fr. Demande, 22 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION: DATENT NIO

PA'	PATENT NO.								APPLICATION NO.									
FR	FR 2865208																	
AU	2005	2128	67		A1	A1 20050825				AU 2	2005-	2128	67	20050107				
CA	2549	954			A1	20050825			1	CA 2	2005-	2549	954	20050107				
WO	2005	0779	55		A1		2005	0825	,	WO 2005-FR27					20050107			
	W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑU,	AZ,	BA,	BB,	, BG,	BR,	BW,	BY,	BZ,	CA,	CH,	
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		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	, MK,	MN,	MW,	MX,	MΖ,	NA,	NI,	
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EP	1709	052			A1	20061011				EP 2	2005-	7173	75		2	0050	107	
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BR	2005 2007	0068	79		А	20070612				BR 2005-6879								
							2007			JP 2006-548338			20050107					
	IN 2006KN01850						0511		IN 2006-KN1850									
	US 20070155749				20070705				US 2006-456345									
	MX 2006PA07984					2006			MX 2006-PA7984									
	2007									KR 2006-714266								
	2006				A		2006	1011						20060814				
PRIORIT	RIORITY APPLN. INFO.:										2004-						-	
										WO 2	2005-1	FR27		Ī	W 2	0050	107	

OTHER SOURCE(S): MARPAT 143:133407

858628-83-8P, 3-[(1,4-Diazabicyclo[3.2.1]oct-4-yl)carbonyl]-6methyl-1H-pyrazolo[3,4-b]pyridine dihydrobromide 858628-85-0P,

3-[(1,4-Diazabicyclo[3.2.1]oct-4-yl)carbonyl]-1H-indazole monohydrochloride 858628-87-2P, 6-Chloro-3-[(1,4diazabicyclo[3.2.1]oct-4-yl)carbonyl]-1H-indazole monohydrobromide 858628-89-4P, 3-[(1,4-Diazabicyclo[3.2.1]oct-4-yl)carbonyl]-5fluoro-1H-indazole dihydrobromide 858628-91-8P 858628-94-1P 858628-96-3P 858628-98-5P 858629-01-3P 858638-38-7P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (nicotinic receptor α 7 subunit ligand; preparation of 1,4-diazabicyclo[3.2.1]octanecarboxamides as ligands for nicotinic receptors, especially $\alpha 4\beta 2$ and $\alpha 7$ subunits, for treating central nervous system diseases) 858628-83-8 CAPLUS RN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(6-methyl-3H-pyrazolo[3,4-CN b]pyridin-3-yl)-, hydrobromide (1:2) (CA INDEX NAME)

•2 HBr

RN 858628-85-0 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl-1H-indazol-3-yl-, hydrochloride (1:1) (CA INDEX NAME)

$$\begin{array}{c|c} H \\ N \\ O \\ \end{array}$$

● HCl

RN 858628-87-2 CAPLUS

CN Methanone, (6-chloro-1H-indazol-3-yl)-1,4-diazabicyclo[3.2.1]oct-4-yl-, hydrobromide (1:1) (CA INDEX NAME)

• HBr

RN 858628-89-4 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(5-fluoro-1H-indazol-3-yl)-, hydrobromide (1:2) (CA INDEX NAME)

•2 HBr

RN 858628-91-8 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(6-methyl-3H-indazol-3-yl)-, hydrobromide (1:?) (CA INDEX NAME)

•x HBr

RN 858628-94-1 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl[5-[(methylsulfonyl)oxy]-1H-indazol-3-yl]-, ethanedioate (1:?) (CA INDEX NAME)

CM 1

CRN 858628-93-0 CMF C15 H18 N4 O4 S

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ Me - S - O \\ & & \\ & & \\ O \end{array}$$

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 858628-96-3 CAPLUS

CN Methanone, (5-chloro-1H-indazol-3-yl)-1,4-diazabicyclo[3.2.1]oct-4-yl-(CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & \\ & & \\ & & \\ \end{array}$$

RN 858628-98-5 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(5-methoxy-1H-indazol-3-yl)-(CA INDEX NAME)

$$\begin{array}{c|c} H \\ N \\ O \\ \end{array}$$

RN 858629-01-3 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl-3H-pyrazolo[3,4-b]pyridin-3-yl-, ethanedioate (1:?) (CA INDEX NAME)

CM 1

CRN 858629-00-2 CMF C13 H15 N5 O

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 858638-38-7 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(6-methyl-3H-pyrazolo[3,4-b]pyridin-3-yl)-, hydrochloride (1:?) (CA INDEX NAME)

●x HCl

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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$$C \equiv C - Ph$$

I

AB Title compds. I [D = 0, S, N(R1)2; E = C(R1)2C(R1)2, CR1=CR1, C(R1)2O, etc.; G = 5- or 6-membered aromatic or heteroarom. ring; R1 = H, halo, alkyl, etc.] and their pharmaceutically acceptable salts were prepared For example, coupling of phenylpropynoic acid and 1,4- diazabicyclo[3.2.1]octane dihydrochloride afforded ethanopiperazine II. In nicotinic receptor $\alpha 7$ affinity binding assays, compds. I exhibited specific binding of 75% (sic). ACCESSION NUMBER: 2005:588985 CAPLUS

DOCUMENT NUMBER: 143:115572

TITLE: Preparation of 1,3-ethanopiperazines as nicotinic

acetylcholine receptor ligands

INVENTOR(S): Ernst, Glen; Frietze, William; Jacobs, Robert;

Phillips, Eifion

PATENT ASSIGNEE(S): Astrazeneca AB, Swed. SOURCE: PCT Int. Appl., 23 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PA:	FENT	NO.			KIN	D	DATE			APPI	LICAT	ION	NO.		D.	ATE	
	WO	2005	 0615	 11		A1	_	2005	0707		WO 2	2004-	 SE19	 42		2	 0041	220
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	US	2007	0244	097		A1		2007	1018		US 2	2007-	5835	85		2	0070	410
PRIO:	RIT	Y APP	LN.	INFO	.:						US 2	2003-	5316	44P		P 2	0031	222
											WO 2	2004-	SE19	42		W 2	0041	220

OTHER SOURCE(S): MARPAT 143:115572 IT 857334-56-6P 857334-57-7P 857334-58-8P

857334-59-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of ethanopiperazines as nicotinic acetylcholine receptor ligands)

RN 857334-56-6 CAPLUS

CN 2-Propyn-1-one, 1-(1,4-diazabicyclo[3.2.1]oct-4-yl)-3-phenyl- (CA INDEX NAME)

RN 857334-57-7 CAPLUS

CN 2-Propen-1-one, 1-(1,4-diazabicyclo[3.2.1]oct-4-yl)-2-fluoro-3-phenyl-, (2Z)- (CA INDEX NAME)

Double bond geometry as shown.

RN 857334-58-8 CAPLUS

CN 2-Propen-1-one, 1-(1,4-diazabicyclo[3.2.1]oct-4-yl)-3-(2-methylphenyl)-, (2E)- (CA INDEX NAME)

Double bond geometry as shown.

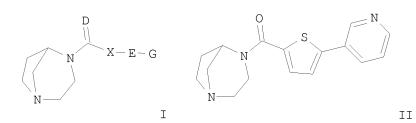
RN 857334-59-9 CAPLUS

CN Ethanone, 1-(1,4-diazabicyclo[3.2.1]oct-4-y1)-2-phenoxy- (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN GI



AB Title compds. I [D = 0, S, N(R1)2; X = Ar1; Ar1 = 5- or 6-membered aromatic or heteroarom. ring with provisos; E = single bond, O, S, etc.; G = H, alkoxy, 5- or 6-membered aromatic or heteroarom. ring, etc.;] and their pharmaceutically acceptable salts were prepared For example, coupling of 1,4-diazabicyclo[3.2.1]octane dihydrochloride and 5-(2-pyridyl)thiophene-2-

carboxylic acid afforded ethanopiperazine II in 60% yield. In nicotinic receptor $\alpha7$ affinity binding assays, compds. I exhibited specific binding of 75% (sic).

ACCESSION NUMBER: 2005:588983 CAPLUS

DOCUMENT NUMBER: 143:115571

TITLE: Preparation of 1,3-ethanopiperazines as nicotinic

acetylcholine receptor ligands

INVENTOR(S): Ernst, Glen; Frietze, William; Jacobs, Robert;

Phillips, Eifion

PATENT ASSIGNEE(S): Astrazeneca AB, Swed. SOURCE: PCT Int. Appl., 40 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

(CA INDEX NAME)

PATENT INFORMATION:

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PATENT NO.
                              KIND DATE
                                                       APPLICATION NO.
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      WO 2005061510
                                A1 20050707 WO 2004-SE1941
                                                                                     20041220
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      JP 2007515479
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                                                                                     20041220
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A 20071025 US 2007-583576
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      US 20070249588
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PRIORITY APPLN. INFO.:
                                                        US 2003-531710P
                                                        WO 2004-SE1941 W 20041220
                               CASREACT 143:115571; MARPAT 143:115571
OTHER SOURCE(S):
      857334-62-4P 857334-63-5P 857334-64-6P
ΙT
      857334-65-7P 857334-66-8P 857334-67-9P
      857334-68-0P 857334-69-1P 857334-70-4P
      857334-71-5P 857334-72-6P 857334-73-7P
      857334-74-8P 857334-75-9P 857334-76-0P
      RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
      (Uses)
          (preparation of ethanopiperazines as nicotinic acetylcholine receptor
          ligands)
RN
      857334-62-4 CAPLUS
      Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl[5-(3-pyridinyl)-2-thienyl]-
CN
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RN 857334-63-5 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(5-phenyl-2-thienyl)- (CA INDEX NAME)

RN 857334-64-6 CAPLUS

CN Methanone, [5-(4-chlorophenyl)-2-furanyl]-1,4-diazabicyclo[3.2.1]oct-4-yl-(CA INDEX NAME)

RN 857334-65-7 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(5-phenyl-2-furanyl)- (CA INDEX NAME)

RN 857334-66-8 CAPLUS

CN Methanone, 2-benzofuranyl-1,4-diazabicyclo[3.2.1]oct-4-yl- (CA INDEX NAME)

$$\begin{array}{c|c} O & C & N \end{array}$$

RN 857334-67-9 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(1-methyl-1H-indol-2-yl)- (CA

INDEX NAME)

RN 857334-68-0 CAPLUS

CN Methanone, [1,1'-biphenyl]-3-yl-1,4-diazabicyclo[3.2.1]oct-4-yl- (CA INDEX NAME)

RN 857334-69-1 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl(4-methoxyphenyl)- (CA INDEX NAME)

RN 857334-70-4 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl-1H-indol-5-yl- (CA INDEX NAME)

RN 857334-71-5 CAPLUS

CN Methanone, 1,4-diazabicyclo[3.2.1]oct-4-yl-2-naphthalenyl- (CA INDEX NAME)

RN 857334-72-6 CAPLUS

CN Benzamide, 4-[5-[(1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-ylcarbonyl]-2-thienyl]-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 857334-73-7 CAPLUS

CN Benzamide, 3-[5-[(1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-ylcarbonyl]-2-thienyl]-N,N-dimethyl- (CA INDEX NAME)

Absolute stereochemistry.

RN 857334-74-8 CAPLUS

CN Methanone, (1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-yl(5-phenyl-2-oxazolyl)-, hydrochloride (1:1) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 857334-75-9 CAPLUS

CN Methanone, (1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-y1[5-(3-pyridinyl)-2-oxazolyl]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry.

●2 HC1

RN 857334-76-0 CAPLUS

CN Methanone, (1R,5R)-1,4-diazabicyclo[3.2.1]oct-4-yl[5-(4-pyridinyl)-2-oxazolyl]-, hydrochloride (1:2) (CA INDEX NAME)

Absolute stereochemistry.

•2 HCl

REFERENCE COUNT:

THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN GI

Ι

AB Title compds. [I; R = alkoxy, halo; R1, R2 = H, alkyl, cycloalkyl,

tetrahydropyran-4-yl; R1R2N = (substituted) 2-oxa-5azabicyclo[2.2.1]heptyl, 3-endo-hydroxy-8-azabicyclo[3.2.1]octyl,
2-azabicyclo[2.2.2]octyl, 1-oxo-2,8-diazaspiro[4.5]decyl,
3-azaspiro[5.5]undecyl, 8-azaspiro[4.5]decyl, 1-oxa-8-azaspiro[4.5]decyl,
1,8,8-trimethyl-3-azabicyclo[3.2.1]octyl, 1,4-oxazepanyl,
2-oxa-5-azabicyclo[2.2.2]octyl, 8-oxa-3-azabicyclo[3.2.1]octyl,
1,4-diazabicyclo[3.2.1]octyl, 2-azabicyclo[2.2.1]heptyl,
3-azabicyclo[3.2.1]octyl, piperazinyl, piperidin-1-yl; X = 0, CH2; n =
0-4], were prepared Thus, 4-methoxy-7-morpholin-4-ylbenzothiazol-2-ylamine
in CH2C12 was treated with pyridine and Ph chloroformate and the resulting
solution stirred for 45 min at ambient temperature; (1S,4S)-2-oxa-5azabicyclo[2.2.1]heptane was added and the mixture stirred at ambient
temperature

for 15 min and at 40° for 2.5 h. to give (1S, 4S)-2-oxa-5-azabicyclo[2.2.1]heptane-5-carboxylic acid <math>(4-methoxy-7-morpholin-4-ylbenzothiazol-2-yl)amide. This bound to human A2a receptors with pKi = 8.5.

ACCESSION NUMBER: 2003:472390 CAPLUS

DOCUMENT NUMBER: 139:53026

TITLE: Preparation of ureidobenzothiazoles as adenosine

receptor ligands

INVENTOR(S): Flohr, Alexander; Jakob-Roetne, Roland; Norcross,

Roger David; Riemer, Claus

PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.					KIND DATE		APPLICATION NO.						DATE					
WO	70 2003049741				A1 20030619				WO 2002-EP13761				20021205					
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ΑT	3597	92			Τ					AT 2002-804578								
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PRIORITY APPLN. INFO.:

EP 2001-129228 A 20011210 US 2002-308338 A3 20021203 WO 2002-EP13761 W 20021205

OTHER SOURCE(S): MARPAT 139:53026

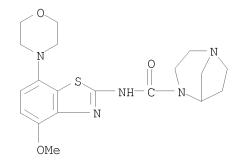
IT 546093-56-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of ureidobenzothiazoles as adenosine receptor ligands)

RN 546093-56-5 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N-[4-methoxy-7-(4-morpholinyl)-2-benzothiazolyl]- (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN GI

AB Four 3-aminopyrrolidine acyl derivs. and 1,4-diazabicyclo[3.2.1]octane-2HCl (I) [5492-61-5] and 2 acyl derivs. were prepared, of which all but I had significant activity in the Litomosoides carinii gerbil test system but had no effect on adult worms. The most active diazabicyclo compound, II [60137-50-0], was prepared from 2-(2-hydroxyethyl)pyrazine [6705-31-3] by hydrogenation, chlorination, ring closure, and acylation. The most active aminopyrrolidine, III [64021-90-5], was prepared from 3-pyrrolidinol [40499-83-0] by acylation, chlorination, reaction with benzylamine, methylation, debenzylation, and methylation. Structure-activity relations are discussed, including the effects of conformation and positions of pharmacophores.

ACCESSION NUMBER: 1977:527018 CAPLUS

DOCUMENT NUMBER: 87:127018

ORIGINAL REFERENCE NO.: 87:20081a,20084a

TITLE: Antifilarial agents. 3-Aminopyrrolidine and

1,4-diazabicyclo[3.2.1]octane derivatives as analogs

of diethylcarbamazine

AUTHOR(S): Sturm, Priscilla A.; Cory, Michael; Henry, David W.;

McCall, J. W.; Ziegler, J. B.

CORPORATE SOURCE: Bio-Org. Chem. Dep., Stanford Res. Inst., Menlo Park,

CA, USA

SOURCE: Journal of Medicinal Chemistry (1977), 20(10), 1333-7

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 87:127018

IT 60137-49-7P 60137-50-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

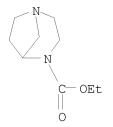
BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and anthelmintic activity of)

RN 60137-49-7 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxylic acid, ethyl ester,

monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 60137-50-0 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N,N-diethyl-,
monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L3 ANSWER 7 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

AB One cis- and 7 trans-1,2-cyclobutanediamines with N-methyl and N-acyl substituents were prepared by monoacylating the appropriate diamine followed by reductive methylation. None of the compds. was active against Litomosoides carinii in the gerbil. Inactivity is discussed in terms of pharmacophore configurations. Structure-activity relations for 24 addnl. diethylcarbamazine [90-89-1] analogs are discussed.

ACCESSION NUMBER: 1977:527003 CAPLUS

DOCUMENT NUMBER: 87:127003

ORIGINAL REFERENCE NO.: 87:20077a,20080a

TITLE: Antifilarial agents. 1,2-Cyclobutanediamines as

analogs of diethylcarbamazine. Status of

structure-activity relations among diethylcarbamazine

analogs

AUTHOR(S): Sturm, Priscilla A.; Cory, Michael; Henry, David W.;

McCall, J. W.; Ziegler, J. B.

CORPORATE SOURCE: Coll. Vet. Med., Univ. Georgia, Athens, GA, USA

SOURCE: Journal of Medicinal Chemistry (1977), 20(10), 1327-33

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

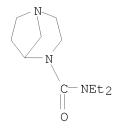
IT 63574-73-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

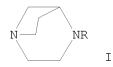
(anthelmintic activity of, structure in relation to)

RN 63574-73-2 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane-4-carboxamide, N,N-diethyl- (CA INDEX NAME)



L3 ANSWER 8 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN GI



AB Diazabicyclooctanes (I; R = EtoCo, Et2NCO), useful as antifilarial agents as indicated by tests against Litomosoides carinii in gerbils, were prepared by acylation of I (R = H) (II) with EtoCoCl and Et2NCoCl; the compds. were isolated as HCl salts. II was prepared by hydrogenating 2-(2-hydroxyethyl)pyrazine with PtO2 catalyst, treating the product with SOCl2, and cyclizing the resultant 2-(2-chloroethyl)piperazine with aqueous NaOH.

ACCESSION NUMBER: 1976:494404 CAPLUS

DOCUMENT NUMBER: 85:94404

ORIGINAL REFERENCE NO.: 85:15129a,15132a

TITLE: 1,4-Diazabicyclo[3.2.1]octanes
INVENTOR(S): Henry, David W.; Sturm, Priscilla A.
PATENT ASSIGNEE(S): Stanford Research Institute, USA

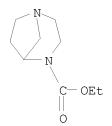
SOURCE: U.S., 3 pp. CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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	US 3954766	A	19760504	US 1975-594510		19750709				
PRIO	RITY APPLN. INFO.:			US 1975-594510	Α	19750709				
ΙT	60137-49-7P 60137-50-0P									
	RL: SPN (Synthetic preparation); PREP (Preparation)									
	(preparation of, for use as antifilarial agent)									
RN	60137-49-7 CAPLUS									
CN	1,4-Diazabicyclo[3.2.1]octane-4-carboxylic acid, ethyl ester,									
	monohydrochloride (9CI) (CA INDEX NAM	E)						



● HCl

● HCl

L3 ANSWER 9 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN AΒ Lactonization of the stereoisomeric N-(carboxymethyl)-4-phenyl-4ethylpyrrolidin-3-ols as well as of the corresponding Me and Et esters and of their 3-acetates afforded the bicyclic lactone, 6-phenyl-6-ethyl-1-aza-4-oxabicyclo[3.2.1]octan-3-one. Reductive cyclization of N-(carbethoxymethyl)-2-phenyl-2-ethylpyrrolidin-3-one oxime yielded the bicyclic lactam, 8-phenyl-8-ethyl-1,4-diazabicyclo-[3.2.1]octan-3-one. ACCESSION NUMBER: 1972:113167 CAPLUS DOCUMENT NUMBER: 76:113167 ORIGINAL REFERENCE NO.: 76:18277a,18280a TITLE: Bridged bicyclic compounds. 6-Phenyl-6-ethyl-1-aza-4-

TITLE: Bridged bicyclic compounds. 6-Phenyl-6-ethyl-1-aza-4-oxabicyclo[3.2.1]octan-3-one and 8-phenyl-8-ethyl-1,4-

diazabicyclo[3.2.1]octan-3-one

AUTHOR(S): Hirshfeld, A.; Taub, W.; Glotter, E.

CORPORATE SOURCE: Dep. Chem., Weizmann Inst. Sci., Rehovot, Israel

SOURCE: Tetrahedron (1972), 28(5), 1275-87

CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 76:113167

IT 35729-86-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 35729-86-3 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane, 4-acetyl-8-ethyl-8-phenyl-, compd. with

2,4,6-trinitrophenol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 46939-11-1 CMF C16 H22 N2 O

CM 2

CRN 88-89-1 CMF C6 H3 N3 O7

3

L3 ANSWER 10 OF 10 CAPLUS COPYRIGHT 2008 ACS on STN

AB 2-(2-Chloroethyl)piperazine (I) was treated with NaOH to give 1,3-ethanopiperazine (II), which was possibly acylated or alkylated at the 4-C. Thus, 10 g. 2-(2-hydroxyethyl)pyrazine was hydrogenated in 150 cc.

MeOH at room temperature, under a H pressure of 2.8 kg./cm.2, in the presence of

2.5 g. Pt20 for 20 hrs., filtered off, and the filtrate distilled in vacuo to give a residue of 2-(2-hydroxyethyl)piperazine (III), which gave by reaction with an excess of HCl in MeOH, a precipitate of III.2HCl, m. .apprx.210°. SOCl2 (100 cc.) was added at -40° in 3-cc.

portions to 20 g. III. The reaction mixture was refluxed 5.5 hrs., cooled to room temperature, and filtered. The residue was dried to give after precipitation

from acetone I.2HCl (IV), m. $348-50^{\circ}$. A suspension of 60 g. IV in 45 cc. water was cooled and treated with 45 g. NaOH in 45 cc. water. The mixture was extracted 5 times with CHCl3, and the exts. were dried over Na2SO4 and evaporated in vacuo. The residue was distilled in the presence of NaOH at

mm. and $<100^{\circ}$ to give II. Reaction of II with excess HCl in MeOH

yielded II.2HCl, m. 348° . A solution of 0.5 g. II in 3 cc. 10% NaOH solution was treated with 5 times 0.2 cc. BzCl. The solution was extracted 3 times

with 5 cc. CHCl3. The exts. were dried on Na2SO4, evaporated in vacuo, and crystallized 2 times from ether, to give the 4-benzoyl homolog of II (V), m. $95-7^{\circ}$. MeI (14.2 g.) was added slowly with stirring to a solution of 11.3 g. II in 15 cc. acetone, and the mixture refluxed 2 hrs. and dried in vacuo. An aqueous alkaline solution of the residue was extracted 5 times with

CHCl3. The exts. were dried over Na2SO4, evaporated, and distilled in vacuo. The fraction b20 $67\text{--}70^\circ$ was the 4-methyl homolog of II (VI). II,

V, and VI are veterinary anthelmintics.

ACCESSION NUMBER: 1966:27623 CAPLUS

DOCUMENT NUMBER: 64:27623 ORIGINAL REFERENCE NO.: 64:5115d-g

TITLE: 1,3-Ethanopiperazine and derivatives

PATENT ASSIGNEE(S): Merck & Co., Inc.

SOURCE: 9 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

10 cc.

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE					
	NL 6501367		19650804	NL 1965-1367	19650203					
	US 3281423			US						
PRIC	RITY APPLN. INFO.:			US	19640203					
ΙT	IT 5167-10-2P, 1,4-Diazabicyclo[3.2.1]octane, 4-benzoyl-									
	RL: PREP (Preparati	on)								

(preparation of)

RN 5167-10-2 CAPLUS

CN 1,4-Diazabicyclo[3.2.1]octane, 4-benzoyl- (7CI, 8CI) (CA INDEX NAME)

$$\begin{array}{c|c} N \\ N \\ C-Ph \\ \parallel \\ O \end{array}$$

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